CLAIMS

What Is Claimed Is:

- 1 1. A method comprising:
- 2 predicting a secondary structure of a protein;
- 3 superimposing the predicted secondary structure on a set of topomers;
- 4 refining the superimposed secondary structure; and
- 5 predicting a tertiary structure of a protein
- 1 2. The method of claim 1, wherein said secondary structure is a consensus
- 2 secondary structure prediction.
- 1 3. The method of claim 1, further comprising annealing the secondary structure by
- 2 energy minimization.
- 1 4. The method of claim 3, wherein said energy minimization is by a random
- 2 Monte Carlo method.
- 1 5. The method of claim 4, wherein the random Monte Carlo method uses random
- 2 moves from a log probability table.
- 1 6. The method of claim 3, wherein the random Monte Carlo method uses smart
- 2 moves.
- 1 7. The method of claim 1, wherein the secondary structure superimposed on a set
- 2 of topomers is refined by energy minimization.
- 1 8. The method of claim 7, wherein the secondary structure superimposed on a set
- 2 of topomers is refined using a molecular modeling program.
- 1 9. The method of claim 8, wherein the molecular modeling program is X-PLOR.
- 1 10. A method comprising:
- 2 predicting a secondary structure of a protein;
- 3 generating a three-dimensional representation of the predicted secondary structure;

- 4 optimizing the secondary structure by adjusting dihedral angles using smart moves; and
- 5 determining a three-dimensional protein structure by modeling the optimized secondary
- 6 structure on a topomer model.
- 1 11. The method of claim 10, wherein said secondary structure is a consensus
- 2 secondary structure prediction.
- 1 12. The method of claim 10, wherein optimization is performed using a random
- 2 Monte Carlo method.
- 1 13. The method of claim 12, wherein the random Monte Carlo method is used in
- 2 conjunction with a localized energy function.
- 1 14. The method of claim 10, wherein said three-dimensional structure model is
- 2 refined using simulated annealing.
- 1 15. A machine readable medium that provides instructions, which when executed
- 2 by a machine cause said machine to perform a method comprising:
- 3 predicting a secondary structure of protein;
- 4 superimposing the secondary structure on a topomer model; and
- 5 refining the topomer model.
- 1 16. A machine readable medium as in claim 15, wherein said secondary structure is
- 2 a consensus secondary structure prediction.
- 1 17. A machine readable medium as in claim 15, further comprising energy
- 2 minimization of the secondary structure prediction.
- 1 18. A machine readable medium as in claim 17, wherein said energy minimization
- 2 is by a random Monte Carlo method.
- 1 19. A machine readable medium as in claim 18, wherein random moves are selected
- 2 from a log probability table.

- 1 20. A machine readable medium as in claim 15, wherein the topomer model is
- 2 refined by topological entropy minimization.
- 1 21. A machine readable medium as in claim 20, wherein the topomer model is
- 2 refined by a molecular modeling program.